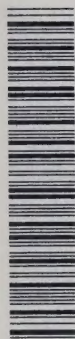


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REPORT: AQRB-81-027-L

Sensitivity Tests

with a

Trajectory Model

by

John L. Walmsley, Jocelyn Mailhot*

and Ronald F. Hopkinson**

March 1981

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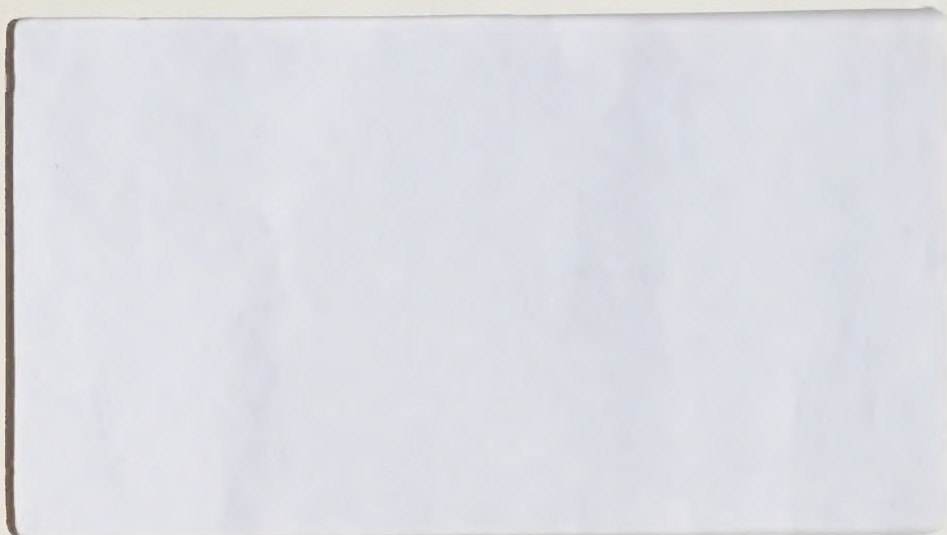


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This is one of a series of internal reports prepared in the Atmospheric Research Directorate. It is an unpublished manuscript.

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Abstract

A method for the derivation of non-divergent wind fields from stream functions which are dependent on latitude and longitude is described. Appropriate choice of seven adjustable parameters enables fairly realistic simulation of frictionless flow. The differential equations for trajectories in these analytically specified flows are solved numerically with a high degree of accuracy, giving a standard against which results from trajectory models may be compared.

This method is used to evaluate the Atmospheric Environment Service (AES) trajectory model for Long-Range Transport of Atmospheric Pollutants (LRTAP). Results showing the effect of the scale of synoptic waves, the size of the timestep, the finite difference scheme, and the horizontal interpolation on the performance of the AES-LRTAP trajectory model are presented.

ACKNOWLEDGEMENTS

We wish to thank Dr. John Reid and Messrs. Marvin Olson and Ken Oikawa for several useful discussions. We are very grateful to Dr. Peter Taylor for his thorough review of this work and for proofreading the manuscript. This paper was typed by Ms. Evonna Mathis and Ms. Barbara Grogan, to whom we owe our thanks.

1. INTRODUCTION

During the 1960's and early 1970's the solution to local atmospheric pollution problems seemed to be the construction of taller stacks which very effectively reduced ground-level concentrations in the immediate vicinity of the source. Observations of increasing acidity of lakes in southern Norway, however, gave an indication that pollutants were being transported great distances from their point of origin. The long transport times were sufficient to allow chemical transformations to occur, adding further complexity. Thus in the early 1970's the phenomenon of long-range transport of air pollution began to be examined with increasing interest. Studies of transport, transformation and deposition mechanisms have been undertaken and attempts have been made to model these processes. Eliassen (1980) has presented a review of these modelling efforts.

At AES a project on the Long-Range Transport of Air Pollutants (LRTAP) was initiated during the mid-1970's encompassing all of the above mentioned research activities. In particular, a computerized trajectory model was developed for application to the LRTAP project. The model, described by Olson et al. (1978) has been used in conjunction with a concentration/deposition model (Olson et al., 1979) to compute atmospheric concentrations and deposition of pollutants transported over long distances.

To date the accuracy of the trajectory - concentration/deposition model system has been evaluated by comparison with other models and by comparison with observations of pollutant concentration at ground level and/or deposition. In addition, verification of the trajectory model has occasionally been done using correlation spectrometer measurements of vertically integrated sulphur dioxide from the Sudbury Inco plume at distances up to 400 km (Millan and Chung, 1978).

The present study attempts a more direct evaluation of the trajectory model by using specified wind fields rather than

those obtained from the Canadian Meteorological Centre (CMC) by objective analysis of observational data. The wind fields we use are determined by specifying the stream function as a simple, yet fairly realistic, function of latitude and longitude. This method enables us to write differential equations for trajectories which we solve numerically, for a given starting position, with high accuracy. Trajectories produced in this manner are used for verifying the AES trajectory model in a number of sensitivity tests. Furthermore, since our wind fields are continuous functions of space, they may be used to evaluate the accuracy of the horizontal interpolation scheme used in the AES model.

In Section 2 we describe the specification of the wind fields, the choice of the stream function and the solution of the trajectory equations. In Section 3 we obtain some theoretical estimates of errors from various sources. Section 4 describes a number of sensitivity tests with the AES model in which results are compared with the solutions obtained in Section 2.

2. WINDS & TRAJECTORIES USED FOR COMPARISON WITH THE TRAJECTORY MODEL

We consider, for the moment, a situation in which the wind is not a function of height or time. We wish to specify a non-divergent wind field which is both simple and realistic.

2.1 Specification of a Non-Divergent Wind Field

In spherical coordinates the wind field may be defined by:

$$u' = R \cos \phi \frac{d\lambda}{dt} \quad (1)$$

$$v' = R \frac{d\phi}{dt} \quad (2)$$

where (u', v') are the (eastward, northward) components of wind

velocity (km hr^{-1}),

ϕ is latitude (positive in the Northern Hemisphere),

λ is longitude (positive in the Eastern Hemisphere),

R is the radius of the Earth (6371 km),

t is the time (hr).

On a polar stereographic map projection with standard latitude at 60°N we superimpose a Cartesian (x,y) grid with origin at the North Pole and positive x -axis along longitude $-\lambda_G$ (i.e., the Greenwich meridian is located at an angle $+\lambda_G$ to the positive x -axis). In this grid x and y are dimensionless and are defined by:

$$x = \frac{mR \cos \phi}{\Delta X} \cos (\lambda + \lambda_G), \quad (3)$$

$$y = \frac{mR \cos \phi}{\Delta X} \sin (\lambda + \lambda_G), \quad (4)$$

where

$$m = \frac{1 + \sin 60^\circ}{1 + \sin \phi} \quad (5)$$

is the map-scale-factor, and ΔX is the grid spacing, true at 60°N (381 km for the standard CMC grid). Note that $\lambda_G = -10^\circ$ for the standard grid. The relationship between the (x,y) coordinate system and the polar stereographic map projection is illustrated in Figure 1.

Wind components in this grid are defined by:

$$u = \frac{\Delta X}{m} \frac{dx}{dt} = \frac{\Delta X}{m} \dot{x} \quad (6)$$

$$v = \frac{\Delta X}{m} \frac{dy}{dt} = \frac{\Delta X}{m} \dot{y} \quad (7)$$

and have dimensions of km hr^{-1} .

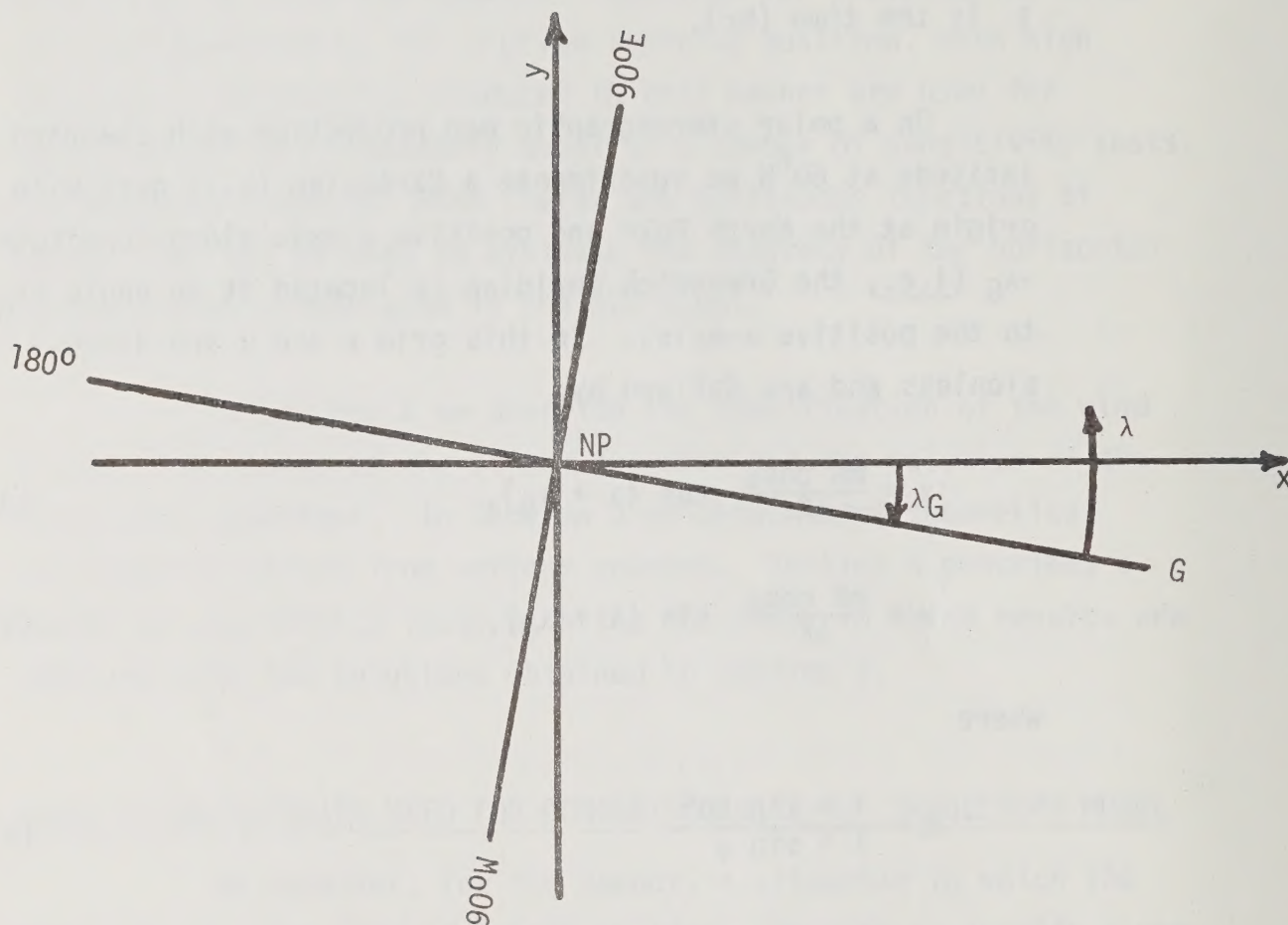


Figure 1. The relationship between the (x,y) coordinate system (positive axes indicated by arrows) and a polar stereographic map projection, (G and NP are the Greenwich Meridian and the North Pole, respectively). In the case of the CMC standard grid, $\lambda_G = -10^\circ$ so the negative y-axis lies along the 80°W Meridian.

Differentiating (3) and (4) with respect to t yields:

$$\begin{aligned} \frac{\Delta X}{R} \frac{dx}{dt} = & -m \left[\cos\phi \sin(\lambda+\lambda_G) \frac{d\lambda}{dt} + \sin\phi \cos(\lambda+\lambda_G) \frac{d\phi}{dt} \right] \\ & + \frac{dm}{dt} \cos\phi \cos(\lambda+\lambda_G) \end{aligned} \quad (8)$$

$$\begin{aligned} \frac{\Delta X}{R} \frac{dy}{dt} = & m \left[\cos\phi \cos(\lambda+\lambda_G) \frac{d\lambda}{dt} - \sin\phi \sin(\lambda+\lambda_G) \frac{d\phi}{dt} \right] \\ & + \frac{dm}{dt} \cos\phi \sin(\lambda+\lambda_G). \end{aligned} \quad (9)$$

It may be shown that:

$$\frac{dm}{dt} = - \frac{m \cos\phi}{1+\sin\phi} \frac{d\phi}{dt}. \quad (10)$$

Therefore, applying (6) and (7) it is possible to derive:

$$u = -R \left[\cos\phi \sin(\lambda+\lambda_G) \frac{d\lambda}{dt} + \cos(\lambda+\lambda_G) \frac{d\phi}{dt} \right] \quad (11)$$

$$v = R \left[\cos\phi \cos(\lambda+\lambda_G) \frac{d\lambda}{dt} - \sin(\lambda+\lambda_G) \frac{d\phi}{dt} \right] \quad (12)$$

Substitution of (1) and (2) then gives:

$$u = - \left[u' \sin(\lambda+\lambda_G) + v' \cos(\lambda+\lambda_G) \right] \quad (13)$$

$$v = u' \cos(\lambda+\lambda_G) - v' \sin(\lambda+\lambda_G). \quad (14)$$

The equation for horizontally non-divergent flow over the surface of a sphere is given by Batchelor (1967):

$$\frac{1}{R \cos\phi} \left[\frac{\partial}{\partial\phi} (v' \cos\phi) + \frac{\partial u'}{\partial\lambda} \right] = 0. \quad (15)$$

If we define a stream function ψ such that:

$$u' = -u_0 \frac{\partial \psi}{\partial \phi} \quad (16)$$

$$v' \cos \phi = +u_0 \frac{\partial \psi}{\partial \lambda} \quad (17)$$

we obtain a (u', v') field which satisfies Eq.(15) and so is horizontally non-divergent. Signs have been chosen so that $u' > 0$ (i.e., eastward) when ψ decreases with increasing latitude. Streamlines are defined by $\psi(\lambda, \phi) = \psi_0$, a constant. Since the flow is steady, trajectories will be along the streamlines. Thus a trajectory which starts at (λ_0, ϕ_0) will be along $\psi_0 = \psi(\lambda_0, \phi_0)$.

Combining Eqs. (1) and (2) with (16) and (17) gives:

$$u' = R \cos \phi \frac{d\lambda}{dt} = -u_0 \frac{\partial \psi}{\partial \phi} \quad (18)$$

$$v' = R \frac{d\phi}{dt} = \frac{+u_0}{\cos \phi} \frac{\partial \psi}{\partial \lambda} \quad (19)$$

Therefore, specification of ψ as a differentiable function of λ and ϕ will yield the wind field (u', v') and differential equations for the trajectory. The grid wind field (u, v) , used by the AES trajectory model is then computed from Eqs. (13) and (14).

2.2 Choice of Stream Function

To our knowledge a realistic example leading to an analytic solution of Eqs. (18) and (19) for trajectory positions $\lambda(t)$ and $\phi(t)$ does not exist. A simple expression for the stream function giving realistic results and leading to a numerical solution can, however, be specified.

2.2.1 Functional Form

An interesting choice is the following:

$$\psi(\lambda, \phi) = \cos^2 \phi [A + B \cos n \lambda + C \cos k(\lambda + \alpha)] - D \sin \phi. \quad (20)$$

Equations (18) and (19) then become:

$$u' = R \cos \phi \frac{d\lambda}{dt} = u_0 \cos \phi [2 \sin \phi (A + B \cos n \lambda + C \cos k(\lambda + \alpha)) + D] \quad (21)$$

$$v' = R \frac{d\phi}{dt} = u_0 \cos \phi [n B \sin n \lambda + k C \sin k(\lambda + \alpha)] \quad (22)$$

This functional form implies zero wind at the poles (where $\phi = \pm 90^\circ$). The set of parameters u_0 , A , B , C , D , n , k and α gives the flexibility necessary to simulate circulations which approximate real situations.

Mean wind components, averaged around a latitude circle are obtained by integrating Equations (21) and (22) with respect to λ from -180° to $+180^\circ$, giving:

$$\overline{u'}^\phi = u_0 \cos \phi [2A \sin \phi + D] \quad (23a)$$

$$\overline{v'}^\phi = 0 \quad (23b)$$

It will prove difficult, if not impossible, to specify A and D in such a way as to obtain realistic mean zonal winds in both Northern and Southern Hemispheres simultaneously. We will assume $\phi > 0$ and merely note that changing the sign of A will give equivalent values of mean zonal winds at corresponding Southern latitudes.

From Equation (23a) it is apparent that $\overline{u'}^\phi = 0$ at the North Pole and when $2A \sin \phi + D = 0$. It is also seen that mean zonal westerlies or easterlies are obtained according to whether $2A \sin \phi + D$ is positive or negative. If both A and D are positive, mean zonal westerlies will exist throughout the Northern Hemisphere. By choosing A and D of opposite sign it is possible to simulate

sub-tropical high pressure regions separating mid- and high-latitude westerlies from Trade-wind zone easterlies. A choice of both A and D negative would result in unrealistic easterlies at all Northern latitudes.

The mean latitude of maxima and minima in $\overline{u'}^\phi$ may be determined by differentiating Equation (23a) and setting the result equal to zero, giving $2A \cos 2\phi = D \sin \phi$. Ignoring the trivial solutions obtained when both A and D are zero, we have $\phi = 45^\circ$ when $D = 0$ and

$$\frac{\sin \phi}{\cos 2\phi} = \frac{2A}{D}, \quad D \neq 0. \quad (24)$$

This may be solved for ϕ by iteration. Northern Hemisphere solutions lie in the following ranges:

$$\begin{aligned} 0^\circ \leq \phi < 30^\circ\text{N} & \quad \text{for} \quad 0 \leq 2A/D < 1, \\ 30^\circ\text{N} \leq \phi < 45^\circ\text{N} & \quad \text{for} \quad 1 \leq 2A/D, \\ \phi = 45^\circ\text{N} & \quad \text{for} \quad D = 0 \\ 45^\circ\text{N} < \phi \leq 90^\circ\text{N} & \quad \text{for} \quad 2A/D \leq -1. \end{aligned}$$

The first two cases represent westerly jet streams provided both A and D are positive (see Equation (23a)). The third case will also be a westerly jet if A is positive. The fourth case will only be a westerly jet if $2A \sin \phi + D > 0$.

The amplitudes of the short- and long-wave components of u' are obtained from Equation (21) and $B u_0 \sin 2\phi$ and $C u_0 \sin 2\phi$, respectively. Both are maximum at $\phi = 45^\circ\text{N}$ where $\sin 2\phi = 1$. The corresponding amplitudes of v' are obtained from Equation 22 as $n B u_0 \cos \phi$ and $k C u_0 \cos \phi$, respectively. These are maximum at the Equator where $\cos \phi = 1$.

2.2.2 Selection of Parameters

As mentioned above, parameters A and D establish a zonal circulation and the position of a jet stream and/or sub-tropical high pressure regions. Values of A and D for two basic flows are given in Table 1a. By an appropriate choice of parameters B, C, n and k one can simulate short waves (synoptic scale and long waves (Rossby waves))superimposed on a zonal circulation as are often observed on constant pressure charts.

The principal function of the different parameters is indicated in Table 1a. By choosing $k = 4$ and $\alpha = 55^\circ$ a circulation marked by a major trough over the centre of the North American continent (100°W) and a ridge over the Maritime Provinces (at $\lambda = -\alpha$ or 55°W) is obtained. The choice of $C = 0.2$ is intended to ensure that the long-wave amplitude of u' is less than $0.2 u_0$ and the corresponding amplitude of v' is less than $0.8 u_0$ at all latitudes (see previous subsection).

Sensitivity of the model to synoptic-scale systems may be evaluated by using $n = 10, 20$ and 40 . Corresponding values of B are $0.1, 0.05$ and 0.03 , respectively, in order to keep $(n B)$ of order 1. Thus the amplitude of both u' and v' short-wave components are kept less than order u_0 . Wavelengths of the short-waves are $36, 18$ and 9 degrees longitude for $n = 10, 20$ and 40 , respectively. At 60°N this would mean wavelengths of $2000, 1000$ and 500 km and at 45°N , $2839, 1415$ and 708 km, respectively. It should be recalled that the grid resolution of the wind data is 381 km.

Some properties of the resulting flows are given in Table 1b, the three values of short-wave amplitudes corresponding to $n = 10, 20$ and 30 , respectively.

Examples of the circulation resulting for each of the two basic flows with $n = 20$ and $k = 4$ are given in Figure 2.

TABLE 1a. PARAMETERS USED FOR THE SENSITIVITY TESTS

PARAMETER	PRINCIPAL FUNCTION	FLOW 1	FLOW 2
u_0	Mean Speed	10 m s^{-1}	10 m s^{-1}
A } and D }	Zonal circulation and mean latitude of jet stream and/or sub-tropical high pressure zone	0.25 1.33	3.5 -3.5
n	Wavenumber of short waves	10, 20, 40	10, 20, 40
B	Maximum amplitude of short-wave zonal wind component	0.1,0.05,0.03	0.1,0.05,0.03
k	Wavenumber of long waves	4	4
C	Maximum amplitude of long-wave zonal wind component	0.2	0.2
α	Phase of long waves	55°	55°

TABLE 1b. PROPERTIES OF THE FLOW

PROPERTY	FLOW 1	FLOW 2
Mean latitude of Jet Stream	17.8°N	57.5°N
Mean latitude of Sub-Tropical High	none	30°N
Short-wave amplitudes at 45°N:		
u'/u_0	0.10, 0.05, 0.03	0.10, 0.05, 0.03
v'/u_0	0.71, 0.71, 0.85	0.71, 0.71, 0.85
Long-wave amplitudes at 45°N		
u'/u_0	0.20	0.20
v'/u_0	0.57	0.57
Mean zonal wind speed at 45°N	1.19 u_0	1.03 u_0
Mean zonal wind speed at mean latitude of jet stream	1.41 u_0	1.29 u_0

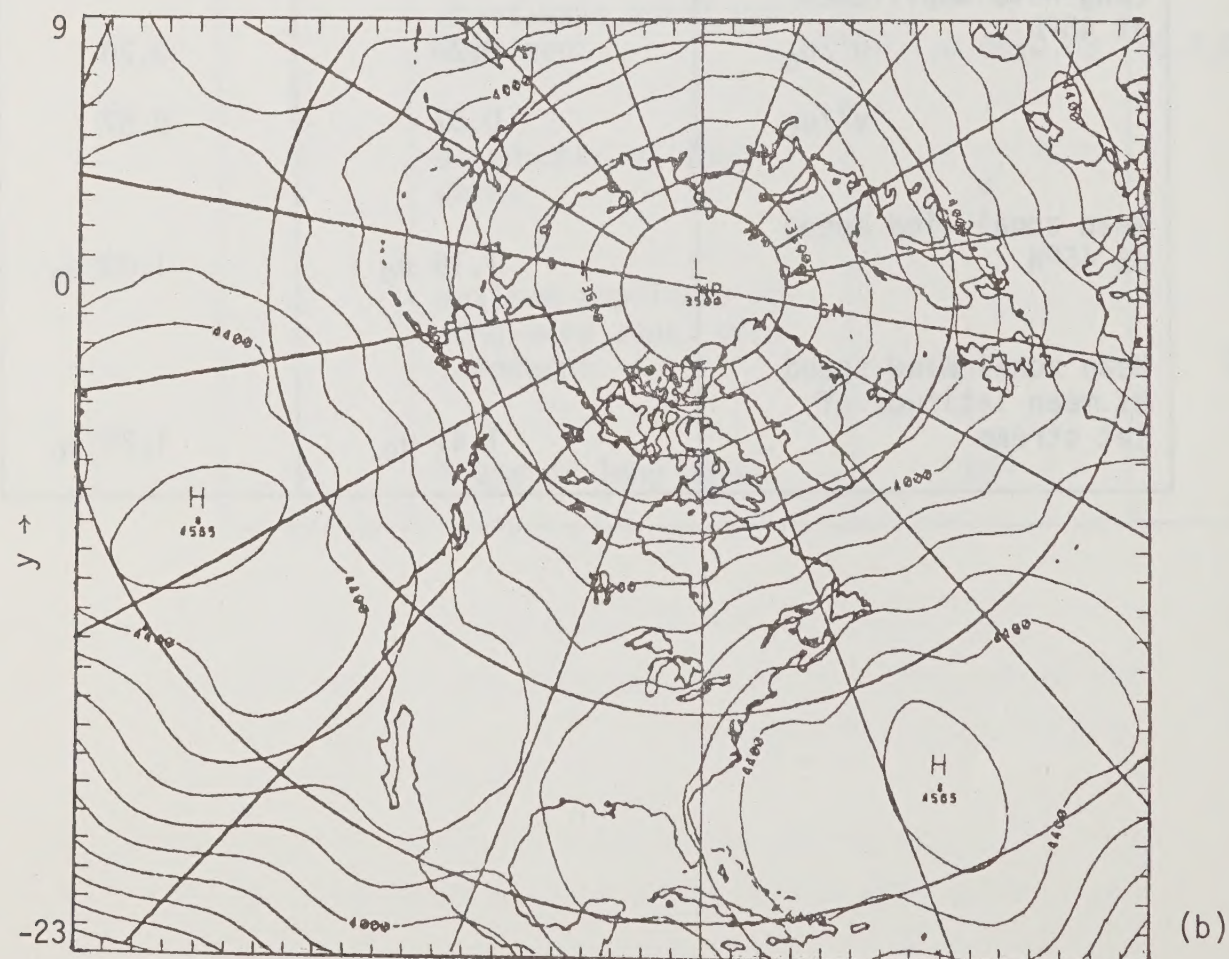
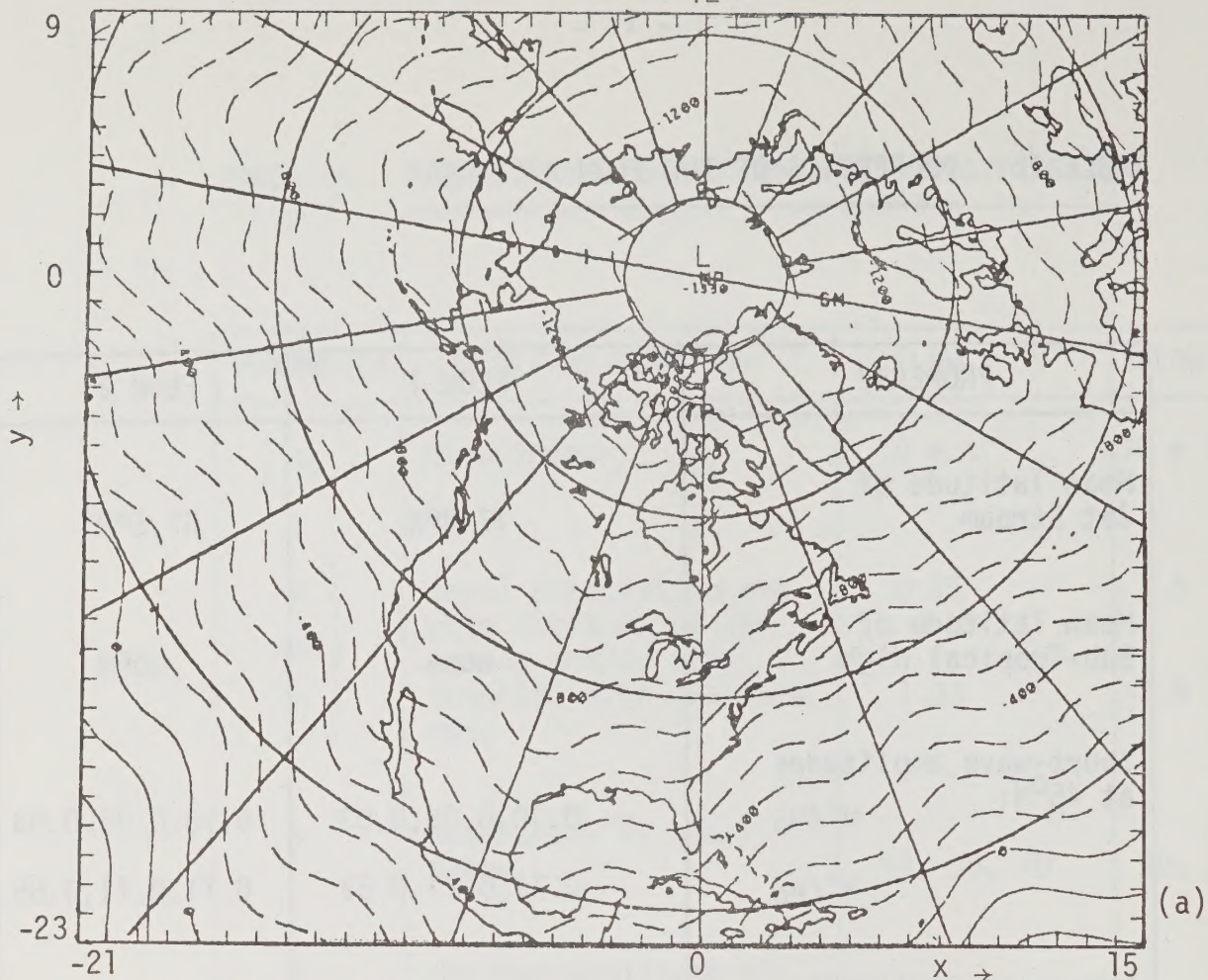


Figure 2. Two examples of the stream function field defined on a 37 x 33 grid of grid size (shown by tick marks) 381 km true at 60°N. Dashed contours represent negative values of ψ . $k = 4$ and $n = 20$.
(a) Flow 1. (b) Flow 2.

2.3 Solution of the Trajectory Equations

The trajectory equations are derived from (21) and (22):

$$\frac{d\lambda}{dt} = \frac{u_0}{R} \left[2 \sin \phi (A+B \cos n \lambda + C \cos k (\lambda+\alpha)) + D \right] \quad (25a)$$

$$\frac{d\phi}{dt} = \frac{-u_0 \cos \phi}{R} \left[n B \sin n \lambda + k C \sin k (\lambda+\alpha) \right] \quad (25b)$$

Given a starting position (λ_0, ϕ_0) , this coupled system of equations is solved numerically for $\lambda(t)$ and $\phi(t)$ using the Hamming Predictor-Corrector method (Ralston and Wilf, 1960) available as a packaged routine on the CYBER 76 computer at CMC. The method is a stable fourth-order procedure. Evaluation of the right-hand-side of the system (25) is required only twice per step, half as many as other methods of the same order of accuracy (e.g., Runge-Kutta). The size of the time increment is automatically adjusted to keep local truncation error within specified limits. The specified maximum time-step could be halved up to ten times in order to achieve the required accuracy, set at $\delta = 10^{-4}$ in the present study. The quantity refers to a weighted deviation between the predicted and corrected values at the i th timestep:

$$\delta = \sum_{j=1}^2 a_j \left[p_j^i - c_j^i \right]$$

where j is the variable index (λ or ϕ); a_j is a weight; p_j^i and c_j^i are the predicted and corrected values, respectively. Taking into account that the zonal component of circulation is usually stronger than the meridional component we have set the weights $a_1 = 0.75$ and $a_2 = 0.25$ for λ and ϕ , respectively. The maximum timestep used is five minutes and the duration of the integration is 42 hours. A supplementary test was performed to verify the accuracy of the numerical method: if (λ_i, ϕ_i) are the values calculated at the i th timestep, then ψ_i obtained from Equation (20) is compared with ψ_0 .

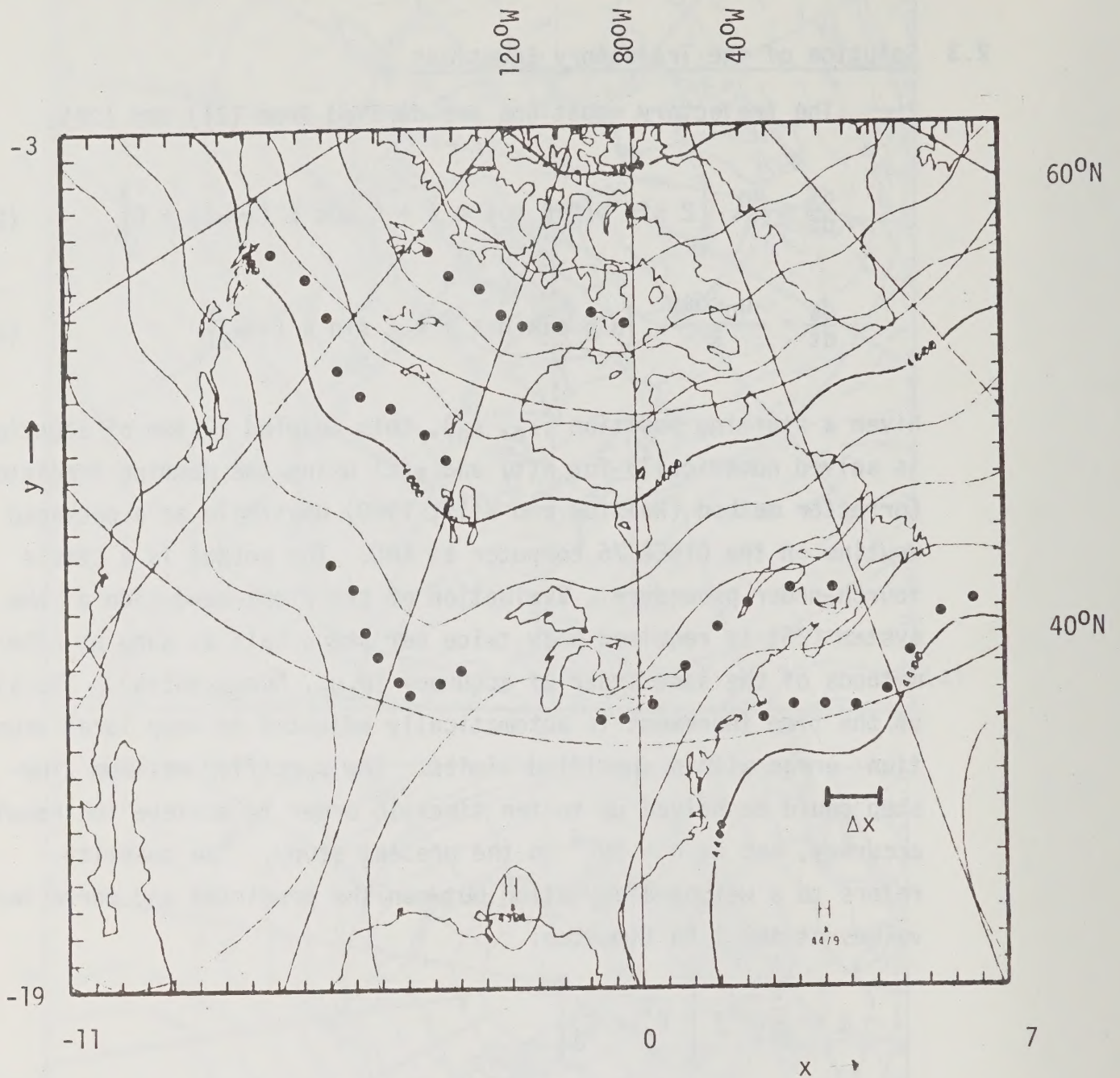


Figure 3. Analytic solution for five trajectories in a Flow 2 simulation with $n = 20$. Positions are shown every 6 hours from 0 to 42 hours. The area shown is a portion of Figure 2b.

Tests showed that relative errors in the values of ψ are less than 10^{-7} .

As an example, Figure 3 shows the solution for five trajectories integrated for 42 hours using the same stream function as in Figure 2b.

3. ESTIMATE OF ERROR IN TRAJECTORY MODELS

3.1 Temporal Truncation Error

Trajectory models obtain numerical solutions to Equations (6) and (7) rearranged as:

$$\frac{dx}{dt} = \dot{x} = \frac{mu}{\Delta X} \quad (26a)$$

$$\frac{dy}{dt} = \dot{y} = \frac{mv}{\Delta X} \quad (26b)$$

For convenience, in the following analysis we will consider only Equation (26a). We will assume, for the moment, that u and v are known exactly at all times and everywhere in the grid. This assumption will permit an examination of the temporal truncation error in finite difference approximations to (26a) without additional sources of error (spatial and temporal interpolation of winds).

We take a Taylor Series expansion of $x(t)$ about $t = t_0$ and evaluate at $t = t_1 = t_0 + \Delta t$, giving:

$$x(t_1) = x(t_0) + (\Delta t) \left. \frac{dx}{dt} \right|_{t_0} + \frac{1}{2} (\Delta t)^2 \left. \frac{d^2x}{dt^2} \right|_{t_0} + O(\Delta t)^3. \quad (27)$$

Equation (27) yields the most straight-forward finite difference approximation:

$$x(t_1) = x(t_0) + \dot{x}(t_0)\Delta t \quad (28)$$

which has an error term:

$$\epsilon = \frac{1}{2} (\Delta t) \left. \frac{d\dot{x}}{dt} \right|_{\zeta} \quad (29)$$

where $x(t_0) \leq \zeta \leq x(t_1)$. The corresponding error in y-position involves the derivative $\dot{y}/dt$.

In order to obtain estimates of combined x- and y-position error, we need to make an assumption about the magnitude of the derivatives. For simplicity we assume first that $C = 0$. Differentiating Equation (13) and (14) with respect to t , squaring and adding and substituting for $d\lambda/dt$ from Equation (18) we obtain:

$$\left(\frac{du'}{dt} \right)^2 + \left(\frac{dv'}{dt} \right)^2 = \left[\frac{du'}{dt} - v' \frac{u'}{L} \left(\frac{\pi}{2n} \right) \right]^2 + \left[\frac{dv'}{dt} + u' \frac{u'}{L} \left(\frac{\pi}{2n} \right) \right]^2,$$

where

$$L = \frac{2\pi R \cos}{4n}$$

is the length scale of short-waves (assumed to be one-quarter of the wave-length). Substituting Equations (23a) and (23b) for u' and v' and assuming

$$\frac{du'}{dt} \approx \frac{U U_p}{L} \quad \text{and} \quad \frac{dv'}{dt} \approx 0,$$

we arrive at the estimate:

$$\left[\left(\frac{du'}{dt} \right)^2 + \left(\frac{dv'}{dt} \right)^2 \right]^{1/2} \approx \frac{U}{L} \left[U_p^2 + U^2 \left(\frac{\pi}{2n} \right)^2 \right]^{1/2}$$

where U_p , the characteristic scale of short-wave u-component perturbations is obtained from the B term of Equation (21):

$$U_p = B u_0 \sin 2\phi.$$

and U , the mean zonal wind is given by (23a):

$$U = u_0 \cos \phi \left[2A \sin \phi + D \right] .$$

Finally, we assume in Equations (6) and (7) that

$$\dot{x} \approx \frac{\bar{m}u}{\Delta X} \quad \text{and} \quad \dot{y} \approx \frac{\bar{m}v}{\Delta X}$$

where $\bar{m}$ is a mean value of m during a particular trajectory.

Therefore

$$\begin{aligned} \epsilon &\approx \frac{1}{2} (\Delta t)^2 \frac{\bar{m}}{\Delta X} \left[\left(\frac{du}{dt} \right)^2 + \left(\frac{dv}{dt} \right)^2 \right]^{\frac{1}{2}} \\ &\approx \frac{1}{2} (\Delta t)^2 \frac{\bar{m}}{\Delta X} \frac{U}{L} \left[U_p^2 + U^2 \left(\frac{\pi}{2n} \right)^2 \right]^{\frac{1}{2}} \end{aligned} \quad (30)$$

It should be noted that ϵ is the error after one timestep of length Δt . For a run of K timestep an upper bound on the total error becomes:

$$\epsilon_{TOT} \approx K\epsilon = \frac{T}{\Delta t} \epsilon ,$$

where T is the duration of the trajectory. Hence

$$\epsilon_{TOT} \approx \frac{1}{2} T (\Delta t) \frac{\bar{m}}{\Delta X} \frac{U}{L} \left[U_p^2 + U^2 \left(\frac{\pi}{2n} \right)^2 \right]^{\frac{1}{2}} .$$

If the long-wave component is also included ($C \neq 0$) then the equation may be modified as follows:

$$\epsilon_{TOT} \approx \frac{1}{2} T (\Delta t) \frac{\bar{m}}{\Delta X} U \left[\left(\frac{U_n}{L_n} \right)^2 + \left(\frac{U_k}{L_k} \right)^2 + \frac{\pi}{2} \left(\frac{U}{L_0} \right)^2 \right]^{\frac{1}{2}}$$

where

$$L_0 = 2\pi R \cos \phi / 4 ,$$

$$L_n = L_0 / n ,$$

$$L_k = L_0/k ,$$

$$U_n = B u_0 \sin 2\phi ,$$

$$U_k = C u_0 \sin 2\phi$$

$$\text{and } U = u_0 \cos \phi [2A \sin \phi + D] .$$

A somewhat better finite difference approximation may be obtained if we also take a Taylor Series expansion of $x(t)$ about $t = t_1$ and evaluate $t = t_0$, giving:

$$x(t_0) = x(t_1) - (\Delta t) \left. \frac{dx}{dt} \right|_{t_1} + \frac{1}{2} (\Delta t)^2 \left. \frac{d^2x}{dt^2} \right|_{t_1} + O(\Delta t)^3 . \quad (32)$$

Combining (27) and (32), we obtain:

$$\begin{aligned} x(t_1) = x(t_0) &+ \frac{1}{2} \left[\dot{x}(t_0) + \dot{x}(t_1) \right] (\Delta t) \\ &+ \frac{1}{4} \left[\left. \frac{d\dot{x}}{dt} \right|_{t_0} - \left. \frac{d\dot{x}}{dt} \right|_{t_1} \right] (\Delta t)^2 \\ &+ O(\Delta t)^3 \end{aligned} \quad (33)$$

A "variable acceleration" model (e.g., Daggupaty, 1979) would retain three terms on the right-hand-side of (33), leaving a truncation error of:

$$\epsilon_3 \approx \frac{1}{12} \left[\left. \frac{d^2x}{dt^2} \right|_{t_0} + \left. \frac{d^2x}{dt^2} \right|_{t_1} \right] (\Delta t)^3 + O(\Delta t)^4 . \quad (34)$$

By a similar process to the one used to obtain an estimate of $\dot{x}/dt$ and $\dot{y}/dt$, we obtain

$$\epsilon_3 \approx \frac{1}{6} T (\Delta t)^2 \frac{\bar{m}}{\Delta X} U^2 \left[\frac{U_n}{L_n^2} + \frac{U_k}{L_k^2} + \left(\frac{\pi}{2} \right)^2 \frac{U}{L_0} \right] \quad (35)$$

and an upper bound on the total error during a trajectory of duration T becomes:

$$\epsilon_{3\text{ToT}} \approx \frac{1}{6} \tau (\Delta t)^2 \frac{\bar{m}}{\Delta X} U^2 \left[\frac{U_n}{L_n^2} + \frac{U_k}{L_k^2} + \left(\frac{\pi}{2}\right)^2 + \frac{U}{L_0^2} \right] . \quad (36)$$

A "constant acceleration" model, on the other hand, would retain only two terms in (33), leaving a truncation error of :

$$\epsilon_2 \approx \frac{1}{4} \left[\frac{d\dot{x}}{dt} \Big|_{t_0} - \frac{d\dot{x}}{dt} \Big|_{t_1} \right] (\Delta t)^2 + \epsilon_3 . \quad (37)$$

For the purpose of estimating this error term we assume that the magnitude of the difference of the two derivatives is given by:

$$\frac{d^2\dot{x}}{dt^2} \Big|_{\bar{t}} (\Delta t) \quad \text{where } \bar{t} = (t_0 + t_1)/2.$$

Thus

$$\epsilon_2 \approx \frac{5}{2} \epsilon_3 \quad (38)$$

and

$$\epsilon_{3\text{ToT}} \approx \frac{5}{2} \epsilon_{3\text{ToT}} \quad (39)$$

From Equations (31) and (39), using a subscript to denote the time-step used in the latter, we obtain the ratio:

$$\frac{\epsilon_{\text{ToT}}}{\epsilon_{2\text{ToT}}} = \frac{6}{5} \frac{(\Delta t)}{(\Delta t)_2^2} \left(\frac{L}{U} \right) \quad (40)$$

which, for synoptic scale features ($U = 36 \text{ km hr}^{-1}$ and $L = 1000 \text{ km}$, corresponding to a wavelength of 4000 km) becomes:

$$\frac{\epsilon_{\text{ToT}}}{\epsilon_{2\text{ToT}}} = \frac{100}{3} \frac{(\Delta t)}{(\Delta t)_2^2} \quad (41)$$

and takes a value of unity when

$$t = 0.03 (\Delta t) \quad (42)$$

Thus, if $(\Delta t)_2 = 6$ hr, a timestep $\Delta t = 1.08$ hr would be required in order that the "zero acceleration" scheme achieve the same accuracy as that of "constant acceleration". Alternatively, if $(\Delta t)_2 = \Delta t$ then

$$\frac{\epsilon_{ToT}}{\epsilon_{3ToT}} = \frac{100}{3(\Delta t)} \quad (43)$$

giving a ratio of 5.6 when $\Delta t = 6$ hr. In summary, the constant-acceleration scheme has the following advantages when compared to the zero-acceleration scheme: a timestep about six times as long gives the same accuracy, or an error about one-sixth as large occurs with the same timestep. In practice, the constant acceleration model will require an iterative procedure to obtain $\dot{x}(t_1)$. Experience with the AES model has shown that two iterations are often sufficient to satisfy the convergence criterion (see Section 4.3.2) so that the constant acceleration scheme would offer to be the better of the two methods if computation time is a consideration.

From Equation (39) we obtain an estimate for the ratio of total errors of the variable and constant acceleration models, viz.,

$$\frac{\epsilon_{3ToT}}{\epsilon_{2ToT}} \approx \frac{2}{5} \quad (44)$$

The extra computation time required by the variable acceleration model would, of course have to be weighed against the increased accuracy. It should be noted that the variable acceleration scheme requires a knowledge of d^2x/dt^2 , the evaluation of which may be of

limited accuracy. Other sources of error (due to the interpolation of winds, the objective analysis which produced the wind field and the wind observations themselves) also have to be considered when choosing the most effective finite difference approximation. In Appendix 'A' we estimate actual magnitudes of errors from various sources in order to aid this decision-making process.

At the present time, the AES trajectory model is a "constant acceleration" model in which it is further assumed that the map-scale-factor, m , is a constant during each timestep. This will be a good assumption when the change in $\sin \phi$ during the timestep is small. Thus the finite difference approximation, Equation (33), becomes:

$$x(t_1) = x(t_0) + \frac{1}{2} \frac{m(t_1)}{\Delta X} \left[u(x_0, t_0) + u(x_1, t_1) \right] (\Delta t) \quad (45)$$

in the case of the AES model. The total truncation error, as noted, is given by Equation (39) with the extra error due to the use of $m(t_1)$ rather than $\bar{m}$ given by:

$$\epsilon_m \approx \frac{\Delta m}{\Delta X} U (\Delta t) \quad (46)$$

or

$$\epsilon_{m_{TOT}} \approx \frac{\Delta m}{\Delta X} U T \quad (47)$$

where $\Delta m = m(t_1) - \bar{m}$. Estimates of the magnitude of this error are given in Appendix A.

3.2 Error due to Horizontal Interpolation of Wind Data

This source of error arises from the need to interpolate wind velocity components from grid-points to positions needed by the finite difference approximation to the trajectory equation. For simplicity we consider only one wind component, u , as a function only

of x and we assume that $n(x)$ is a polynomial of degree N such that:

$$n(x) = u(x) \quad (48)$$

for $x = x_0, x_1, x_2, \dots, x_N$. Thus $u(x)$ is approximated by a polynomial of N th degree and the error of the approximation is given by Conte (1965) as:

$$\beta_N(x) = \frac{\psi(x)}{(N+1)!} \left. \frac{d^{N+1} u(x)}{dx^{N+1}} \right|_{\xi} \quad (49)$$

where

$$\psi(x) = (x - x_0)(x - x_1)(x - x_2) \dots (x - x_N) \quad (50)$$

and

$$x_0 \leq \xi \leq x_N \quad (51)$$

We assume:

$$\left. \frac{d^{N+1} u(x)}{dx^{N+1}} \right|_{\xi} = \frac{U_p}{(L_x)^{N+1}} \quad (52)$$

where U_p is a characteristic amplitude of velocity perturbations and L_x is a characteristic horizontal length scale (in dimensionless x -coordinates). Corresponding dimensional coordinates are $x\Delta X$ (see Equation (3)) so we may define a characteristic horizontal length scale:

$$L = L_x \Delta X \quad (53)$$

Assuming $x_0, x_1, x_2, \dots, x_N$ are equally spaced and taking $x = \frac{1}{2}(x_0 + x_1)$, Equation (49) becomes:

$$\beta_N\left(\frac{1}{2}(x_0 + x_1)\right) = \frac{\frac{1}{2}(-\frac{1}{2})(-\frac{3}{2}) \dots (\frac{1}{2}-N)(\Delta x)^{N+1}}{(N+1)!} U_p \left(\frac{\Delta X}{L}\right)^{N+1} \quad (54)$$

which gives

$$\beta_1 = -\frac{1}{8} U_p \left(\frac{\Delta X}{L} \right)^2$$

and

$$\beta_3 = -\frac{5}{128} U_p \left(\frac{\Delta X}{L} \right)^4$$

for linear and cubic interpolation, respectively. The coefficients change to $-1/12$ and $-1/80$, respectively, on averaging $\beta_N(x)$ over the entire interval x_0 to x_N . The effect of this wind interpolation error on the trajectory position may be seen, in the case of the AES model, by inserting $U + \beta_N$ in place of U in Equation (45). Assuming that both points x_0 and x_1 (which are now positions at the beginning and end of a timestep) are mid-way between grid-points then an upper bound on the magnitude of the position error due to wind interpolation is estimated to be:

$$\epsilon_{\beta_N} \approx \frac{\bar{m}}{\Delta X} \left| \beta_N(\frac{1}{2}) \right| (\Delta t) \quad (55a)$$

or, for a trajectory of duration T :

$$\epsilon_{\beta_N \text{ ToT}} \approx \frac{\bar{m}}{\Delta X} \left| \beta_N(\frac{1}{2}) \right| T$$

$$C_N \frac{\bar{m}}{\Delta X} U_p \left(\frac{\Delta X}{L} \right)^{N+1} T, \quad (55b)$$

where C_N is a coefficient.

In the one-dimensional situation we have examined, we had to obtain estimates of derivatives of U with respect to x (Equation 52). In this case U_p is estimated to be the amplitude of the short-

or long-wave component of u' (see Section 2.2.1). When we consider two-dimensions and two wind components, however, the derivative in Equation (52) is replaced by

$$\left[\left(\frac{\partial^{N+1} u}{\partial x^{N+1}} \right)^2 + \left(\frac{\partial^{N+1} u}{\partial y^{N+1}} \right)^2 + \left(\frac{\partial^{N+1} v}{\partial x^{N+1}} \right)^2 + \left(\frac{\partial^{N+1} v}{\partial y^{N+1}} \right)^2 \right]^{\frac{1}{2}}. \quad \text{In this}$$

case, after transformation to (u', v') and (λ, ϕ) , we find that the dominant derivative is $\partial^{N+1} v' / \partial \lambda^{N+1}$. Hence the magnitude of U_p in Equation (55b) is estimated to be the amplitude of the short- or long-wave component of v' , rather than u' . The former are of order n times the latter, making the error estimates an order of magnitude larger.

Estimates of the magnitude of the error in Equation (55b) are given in Appendix 'A'.

3.3 Error due to Temporal Interpolation of Wind Data

Since wind data is not available as a continuous function of time, an interpolation error analogous to that given by Equation (49) may be expressed as

$$\gamma_m(t) = \frac{\psi(t)}{(M+1)!} \left. \frac{d^{M+1} u(t)}{dt^{M+1}} \right|_{\zeta} \quad (56)$$

where M is the degree of the interpolating polynomial,

$$\psi(t) = (t - t_0)(t - t_1) \dots (t - t_M) \quad (57)$$

and $t_0 \leq \zeta \leq t_M$. We assume that

$$\left. \frac{d^{M+1} u(t)}{dt^{M+1}} \right|_{\zeta} = \frac{U_p}{\tau^{M+1}} \quad (58)$$

where U_p is a characteristic amplitude of velocity perturbations
 $\tau = L/U$ is a characteristic synoptic period, L is a characteristic synoptic length scale and U is a characteristic velocity. Assuming that $t_0, t_1, t_2, \dots, t_M$ are times of synoptic observations, equally-shaped at intervals of $T = 6$ hours, then taking $t = \frac{1}{2} (t_0 + t_1)$ and $t_0 = 0$, Equation (56) becomes:

$$\gamma_M \left(\frac{1}{2} \Delta T \right) = \frac{\frac{1}{2} \left(-\frac{1}{2} \right) \left(-\frac{3}{2} \right) \dots \left(\frac{1}{2} - M \right) (\Delta T)^{M+1}}{(M+1)!} U_p \left(\frac{U}{L} \right)^{M+1} \quad (59)$$

which gives

$$1 = -\frac{1}{8} (\Delta T)^2 U_p \left(\frac{U}{L} \right)^2$$

$$2 = +\frac{1}{16} (\Delta T)^3 U_p \left(\frac{U}{L} \right)^3$$

for linear and quadratic interpolation, respectively. The coefficients change to $-1/12$ and 0 , respectively, on averaging $\gamma_M(t)$ over the entire interval to t_M . The effect of this temporal interpolation error on the trajectory position may be seen by inserting $U + \gamma_M$ in place of U in Equation (45). Assuming that both t_0 and t_1 (which are now times at the beginning and end of a timestep) are mid-way between synoptic data points then an upper bound on the magnitude of the position error due to temporal interpolation is estimated to be:

$$\epsilon_{\gamma_M} \approx \frac{\bar{m}}{\Delta X} \left| \gamma_M \left(\frac{1}{2} \Delta T \right) \right| (\Delta t) \quad (60a)$$

or, for a trajectory of duration T :

$$\epsilon_{\gamma_M \text{ To } T} = \frac{\bar{m}}{\Delta X} \left| \gamma_M \left(\frac{1}{2} \Delta T \right) \right| T$$

$$C_M \frac{\bar{m}}{\Delta X} U_p \left(\frac{U \Delta T}{L} \right)^{M+1} T \quad (60b)$$

where C_M is a coefficient.

Estimates of the magnitude of this error are given in Appendix 'A'.

4. SENSITIVITY TESTS

A number of tests were performed in which the AES trajectory model results were compared with solutions obtained from numerical integration of Equations (25a) and (25b) by the Predictor-Corrector Method. In the following sub-sections we examine the effect of the scale of waves in the stream function, the timestep, the finite difference approximation to the trajectory equation and the horizontal interpolation scheme on the accuracy of model results.

We also investigated inaccuracies introduced by the packing of data from 60-bit to 20-bit CDC computer words. It was found that this practice occasionally resulted in relative errors of order 10^{-3} , which were insignificant when compared with other sources of error. Unpacking of data during model execution, however, requires additional computation time which may be avoided whenever sufficient storage space for unpacked data is available.

In the tests described below five forward trajectories of 42-hour duration were computed. In all cases the analytic wind data were independent of height and of time. This means that there are no errors of the type given, for example, by Equation (60). Root-mean-square (r.m.s.) errors were computed using model versus "exact" (i.e., Predictor-Corrector) solutions for all five trajectories at every timestep. Starting positions of the trajectories are given in Table 2.

4.1 Effect of Scale of Waves

The accuracy of the AES model was examined as a function of the wavenumber of the short waves, n (see Table 1a). Results are presented in Figure 4 in comparison with theoretical estimates computed from Equation (39) with values of parameters given in Table 1a. Model calculations were done for Flow 1 ($n = 10$ and 20) and Flow 2 ($n = 20$ and 40) with $k = 4$ in both cases. Agreement between model

TABLE 2 STARTING POSITIONS FOR TRAJECTORIES. GRID-POINT LOCATIONS ARE RELATIVE TO THE NORTH POLE WHICH IS LOCATED AT THE ORIGIN ($x=0$, $y=0$) AND ARE FOR THE STANDARD CMC GRID (SPACING 381 km, TRUE AT 60°N).

TRAJECTORY NUMBER	GRID-POINT		LATITUDE (°N)	LONGITUDE (°W)
	x	y		
1	-4	- 5	66.8	118.7
2	-7	- 5	59.2	134.5
3	-6	-11	46.2	108.6
4	-1	-14	41.6	84.1
5	+2	-14	41.2	71.9

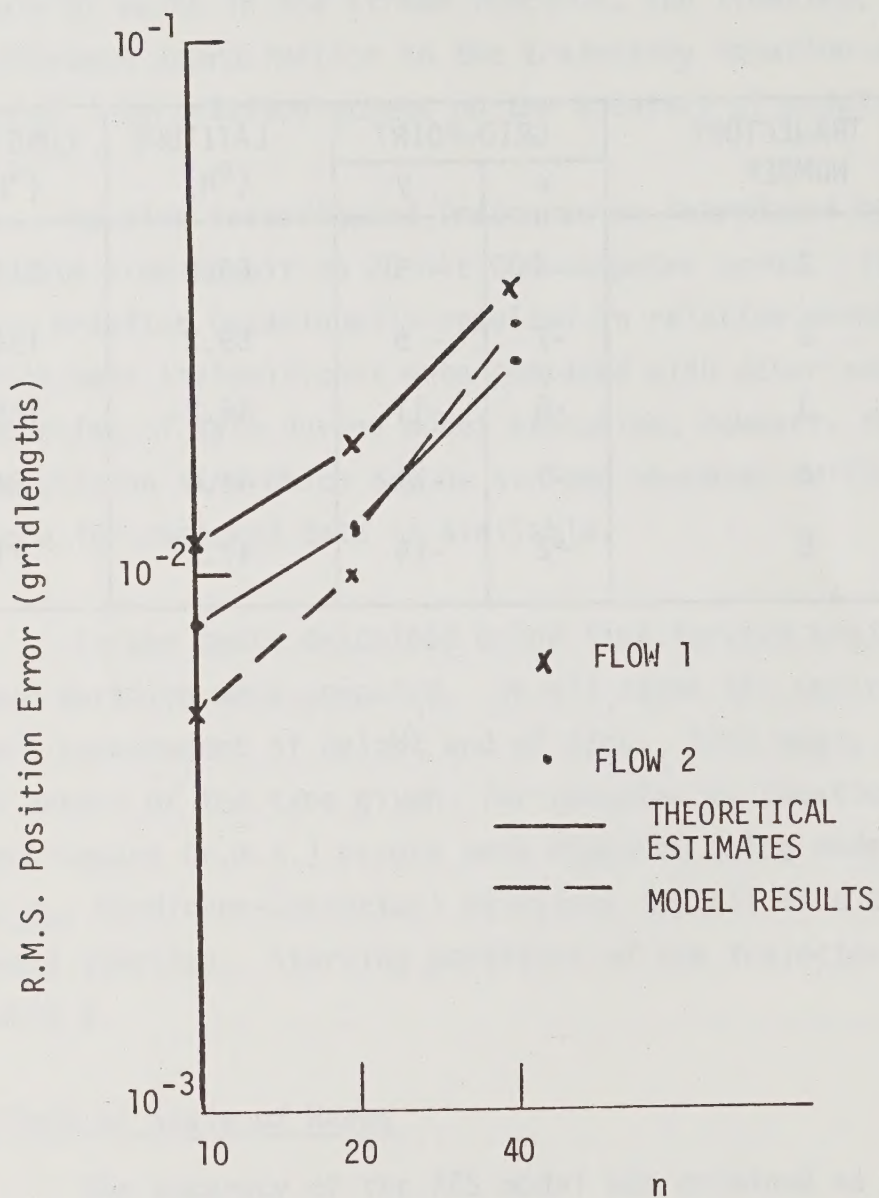


Figure 4. R.M.S. Position error as a function of short-wave wavenumber for two different flow situations with $k = 4$. Error due to wind interpolation has been eliminated.

run results and theoretical estimates is quite good. Slopes of the lines are close to 1, indicating that errors are approximately proportional to n . Examination of Equations (39) and (36) would suggest that, assuming contributions from the mean zonal flow and long-wave components to be negligible, errors are proportional to U_n/L_n^2 , i.e., $n^2 U_n$; however, U_n is proportional to B which is approximately inversely proportional to n . The result is errors approximately proportional to n , departures from a power of unity being due to the presence of long-wave and mean zonal terms and to the fact that B is only approximately inversely proportional to n .

4.2 Effect of Timestep

According to Equation (39), the temporal truncation error in the AES model arising from the finite difference approximation to the trajectory equation is proportional to $(\Delta t)^2$. In order to verify that this is the case, it was decided to run model tests with timesteps of 1, 2, 3 and 6 hours using winds calculated from Equations (13), (14), (21) and (22), thus avoiding interpolation errors. Map-scale-factor errors, Equation (47), were also eliminated for these tests, as they were in Section 4.1 (see Section 4.3.3). Results (which are the same as the 20-wave case in Table 3a) are presented in Table 3a. We also show r.m.s. errors relative to the error with $\Delta t = 6$ hours and compare with $(\Delta t/6)^2$. It can be seen that truncation errors are proportional to $(\Delta t)^2$ as predicted. This relationship is also shown in Figure 5 where results from two different cases we plotted.

Execution times for the above experiments are recorded in Table 3(b). An estimated "overhead" of 3.474 seconds (see Section 4.3) is subtracted and the results show a relationship which is approximately inversely proportional to Δt .

TABLE 3a R.M.S. POSITION ERRORS FOR VARIOUS TIMESTEPS. FLOW 2 WITH 20 CIRCUMPOLAR WAVES IS SIMULATED. RESULTS ARE FOR 5 TRAJECTORIES OF 42-HOUR DURATION. WINDS ARE OBTAINED ANALYTICALLY (i.e., WITHOUT INTERPOLATION ERROR). ERROR DUE TO MAP-SCALE-FACTOR HAS BEEN ELIMINATED.

Timestep Δt (Hours)	RMS Error (Grid Lengths)	$\frac{\text{RMS Error } (\Delta t)}{\text{RMS Error } (6 \text{ hr})}$	$\left(\frac{\Delta t}{6}\right)^2$
1	0.001331	0.027	0.028
2	0.005470	0.110	0.111
3	0.01223	0.246	0.250
6	0.04980	1.000	1.000

TABLE 3b CPU TIMES FOR THE EXPERIMENTS OF TABLE 4a. ESTIMATED "OVERHEAD" IS 3.474 SECONDS.

Timestep Δt (Hours)	CPU Time (Seconds)			$\frac{6}{\Delta t}$
	Total	Without Overhead		
			CPU/CPU (6)	
1	4.550	1.076	6.01	6.00
2	4.035	0.561	3.13	3.00
3	3.838	0.364	2.03	2.00
6	3.653	0.179	1.00	1.00

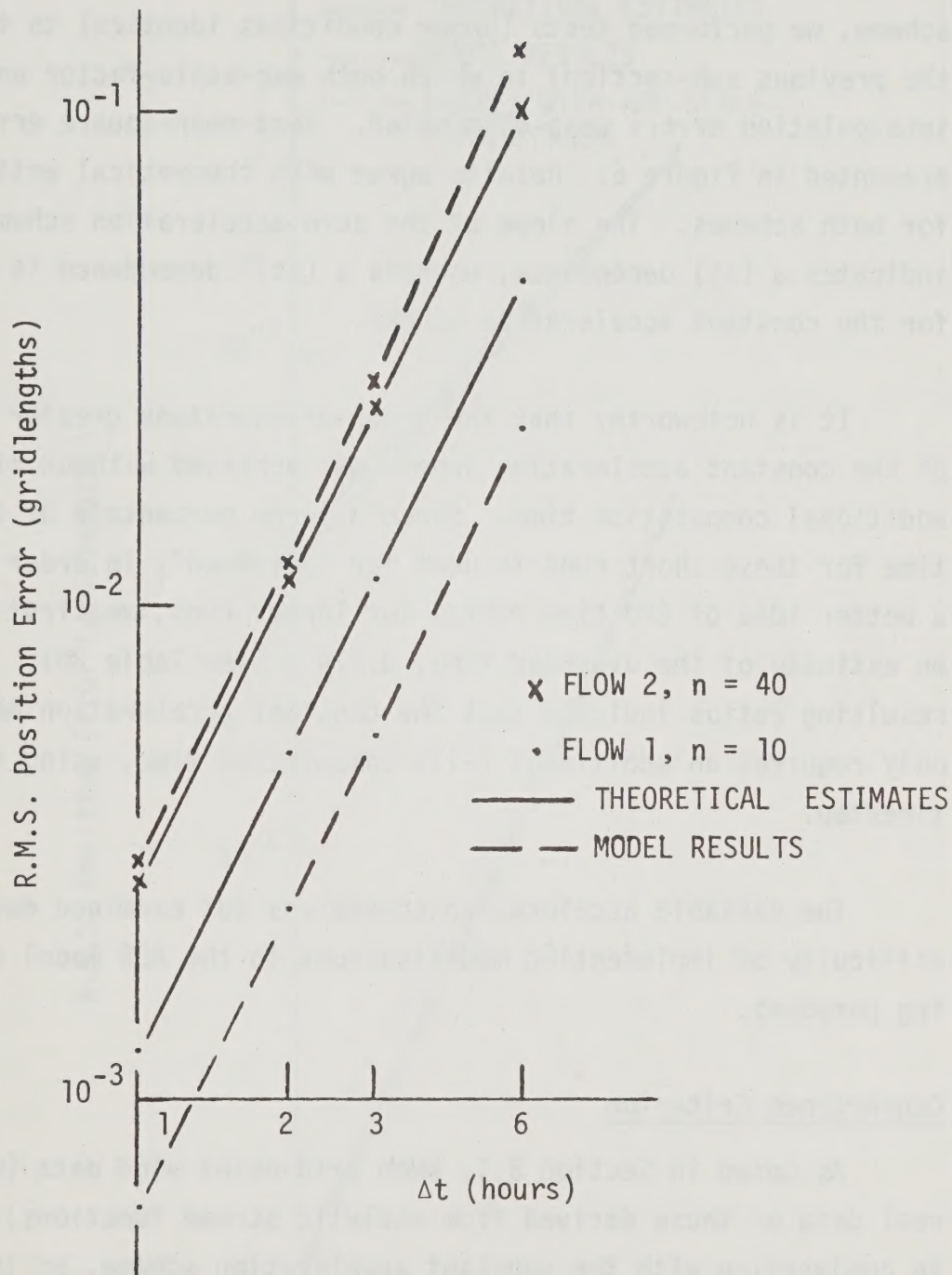


Figure 5. R.M.S. Position Error as a function of timestep for two different flow situations with $k = 4$. Error due to wind interpolation has been eliminated.

4.3 Effect of Finite Difference Scheme

4.3.1 Zero versus Constant Acceleration

In order to compare results from the AES model (constant acceleration) with those from a forward-stepping (zero acceleration) scheme, we performed tests (under conditions identical to those of the previous sub-section) in which both map-scale-factor and wind-interpolation errors were eliminated. Root-mean-square errors are presented in Figure 6. Results agree with theoretical estimates for both schemes. The slope of the zero-acceleration scheme results indicates a (Δt) dependence, whereas a $(\Delta t)^2$ dependence is obtained for the constant acceleration scheme.

It is noteworthy that the order-of-magnitude greater accuracy of the constant acceleration scheme was achieved without significant additional computation time. Since a large percentage of the total time for these short runs is used for "overhead", in order to obtain a better idea of CPU time ratios for longer runs, we first subtracted an estimate of the overhead time, 3.474 s (see Table 3b). The resulting ratios indicate that the constant acceleration method only requires an additional 7-11% computation time, using the same timestep.

The variable acceleration scheme was not examined due to the difficulty of implementing modifications to the AES model for testing purposes.

4.3.2 Convergence Criterion

As noted in Section 3.1, when grid-point wind data (whether real data or those derived from analytic stream functions) are used in conjunction with the constant acceleration scheme, an iterative procedure is required since wind-speed components at the end of the timestep appear on the right-hand side of the finite difference

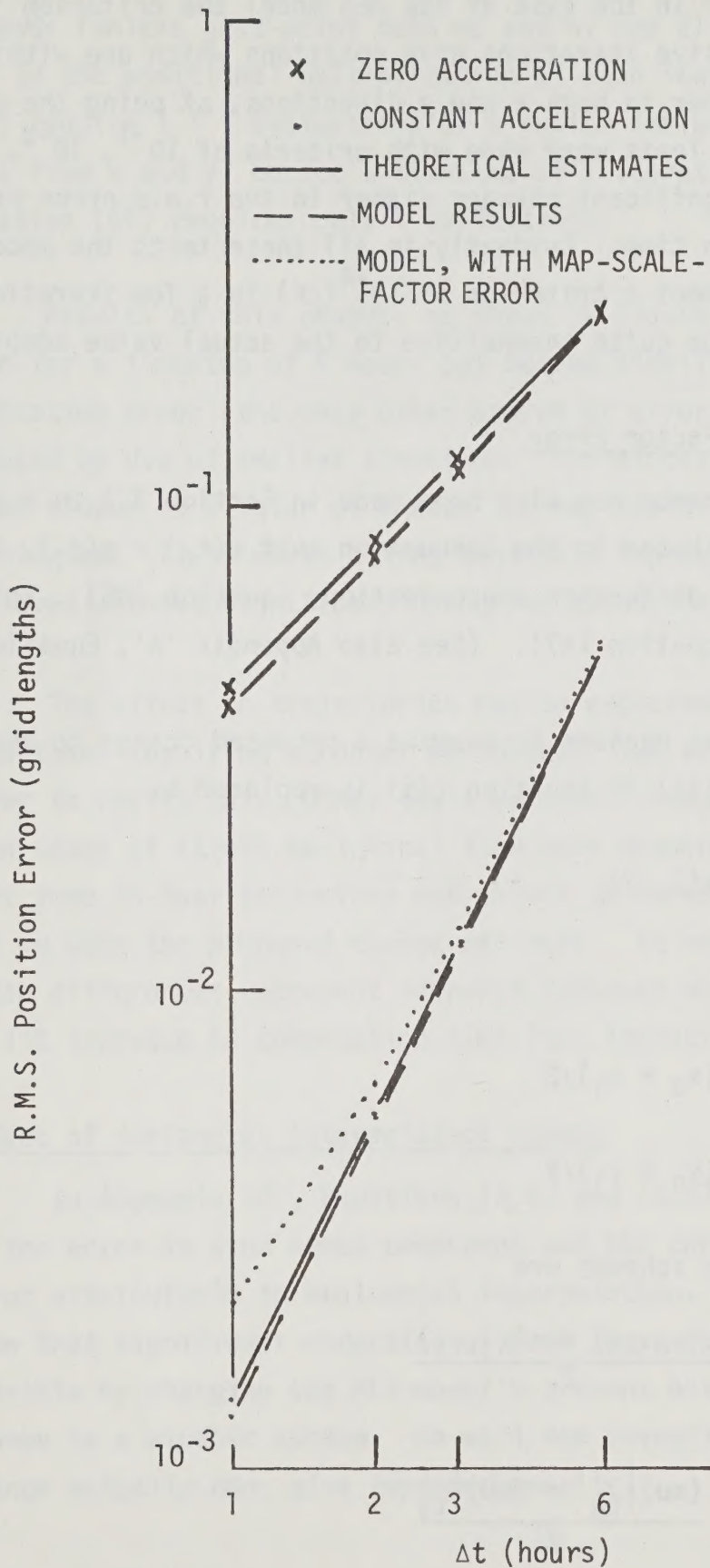


Figure 6. Position errors as a function of timestep for Flow 2 with $n = 20$ and $k = 4$. The zero- and constant acceleration schemes are compared. The effect of the map-scale-factor error is also shown.

approximation. A convergence criterion is needed to end the iteration. In the case of the AES model the criterion is met when two successive iterations give positions which are within $10^{-2}(\Delta X)$ of each other in both x and y directions, ΔX being the grid spacing (381 km). Tests were made with criteria of 10^{-1} , 10^{-3} , $10^{-4}(\Delta X)$ without significant changes either in the r.m.s error or in the computation time. Evidently in all these tests the model must have tended to meet a criterion of $10^{-4}(\Delta X)$ in a few iterations as it proved to be quite insensitive to the actual value adopted.

4.3.3 Map-Scale-Factor Error

Reference has also been made in Section 3.1 to a source of error attributed to the assumption that $m(t_0) = m(t_1)$, leading to the finite difference approximation, Equation (45). This error is given by Equation (47). (See also Appendix 'A', Equation (A.4)).

It was decided to examine a proposed change to the AES model in which $m(t_1)$ in Equation (45) is replaced by

$$\bar{m} = m(\bar{x}, \bar{y}) \quad (61)$$

where

$$\bar{x} = (x_0 + x_1)/2 \quad (62a)$$

$$\bar{y} = (y_0 + y_1)/2 \quad (62b)$$

Alternative schemes are

$$\bar{m} = \frac{m(x_0, y_0) + m(x_1, y_1)}{2} \quad (63)$$

or

$$\bar{m} = \frac{(mu)|_{t_0} + (mu)|_{t_1}}{2} \quad (64)$$

Equation (64) would appear to be the least efficient of the three methods (unless grid-point data μ and ν are already available) due to the additional multiplication at each iteration. Equation (63) require $I + 1$ evaluations of m (which includes determination of ϕ from x and y) during a timestep of I iterations, whereas Equation (61) requires only I evaluations.

Results of this change, as shown in Figure (46) are negligible for a timestep of 6 hours but become significant as the temporal truncation error (the only other source of error in this case) is reduced by use of smaller timesteps. The slopes of the line also comes closer to a value of 2 when the map-scale-factor error is eliminated. It is worth noting that this improvement can be achieved without significant change in execution time.

The effect on trajectories may be expected to increase when situations involving stronger meridional flow are encountered. In order to verify this, other tests were performed using real data. When cases of strong meridional flow were examined, it was found that some 96-hour trajectory end-points differed by as much as 100 km when the proposed change was made. It must be assumed that these differences represent improved accuracy which is achieved by an 11% increase in computation time (see Appendix 'A').

4.4 Effect of Horizontal Interpolation Scheme

In Appendix 'A', Equations (A.6) and (A.8), we obtain estimates of the error in wind speed component and the corresponding position error attributable to horizontal interpolation. In Table A.1 we show that significant reduction of both these errors is theoretically possible by changing the AES model's present bilinear interpolation scheme to a bicubic scheme. We will now investigate whether such a change actually does give improved results.

In Table 4 we present results for several flow simulations, showing bilinear, bicubic and "exact" (labelled L, C, E, respectively) for several different timesteps. Map-scale-factor error has been eliminated in all tests. The "exact" case is the one in which winds are calculated exactly from the analytic formulae, thus eliminating horizontal interpolation error. Any error remaining in the "exact" case is due to the finite difference approximation to the trajectory equation. Results tabulated in Table 6 are the wind speed and wind direction mean biases (compared with the Predictor-Correctory solution) and the standard deviations of individual biases about their respective means. Also included are the r.m.s. position error and the CPU time, both with and without an "overhead" of 3.474 s.

In the Flow 2, 20-wave cases it is clear that the bicubic interpolation scheme gives significant improvements in both wind speed and direction. This is reflected in a substantial decrease in the r.m.s. position error. When timesteps of 3 hours or less are used, the r.m.s. error is reduced by 45 to 50% as a result of using the bicubic scheme, going part way towards the "perfect" results (i.e., without interpolation error) represented by the "exact" case. (Use of a quadratic scheme in one test gave an error close to that obtained by the cubic scheme in about the same CPU time).

In the 40-wave cases some very slight improvements in the wind interpolation is noted, but the increase in accuracy is not as significant as in the 20-wave simulation. Furthermore, the improvement is not reflected in the r.m.s. position error. We must conclude that the waves are so poorly resolved by the grid-point data that even the cubic scheme cannot effect an improvement over the linear one. As noted in Section 4.1, real CMC data would have at most 29 circumpolar waves so that our 40-wave cases are more severe tests than would be encountered with present-day data resolution.

TABLE 4 EFFECT OF HORIZONTAL INTERPOLATION SCHEME ON ERRORS IN WIND VELOCITY AND POSITION. MAP-SCALE-FACTOR ERRORS HAVE BEEN ELIMINATED.

Scheme	Flow	No. Waves	Δt (Hr)	Wind Speed (m s ⁻¹)		Wind Direction (degrees)		RMS Position Error (Grid Lengths)	CPU (seconds)	
				Mean Bias	St.Dev.	Mean Bias	St.Dev.		Total	Without Overhead
L C E	2	20	6	-0.70	1.00	0.17	6.04	0.1922	3.824	0.350
	2	20	6	-0.26	0.59	0.00	4.55	0.1181	4.096	0.622
	2	20	6	-	-	-	-	0.04980	-	-
L C E	2	20	3	-0.72	0.96	0.14	6.12	0.1682	4.035	0.561
	2	20	3	-0.26	0.52	-0.02	4.64	0.09029	4.546	1.072
	2	20	3	-	-	-	-	0.01223	-	-
L C E	2	20	2	-0.71	0.97	0.11	6.16	0.1642	4.261	0.787
	2	20	2	-0.26	0.52	-0.05	4.65	0.08546	4.951	1.477
	2	20	2	-	-	-	-	0.005470	-	-
L C E	2	20	1	-0.72	0.97	0.07	6.20	0.1606	4.761	1.287
	2	20	1	-0.26	0.52	-0.08	4.67	0.08239	5.897	2.423
	2	20	1	-	-	-	-	0.001331	-	-
L C E	2	40	6	-2.30	3.88	-0.96	19.98	0.4056	3.826	0.352
	2	40	6	-2.06	3.82	-1.71	19.71	0.4121	4.136	0.662
	2	40	6	-	-	-	-	0.1298	-	-
L C E	2	40	1	-2.47	3.60	0.68	21.08	0.3612	4.765	1.291
	2	40	1	-2.12	3.46	0.06	20.54	0.3629	5.903	2.429
	2	40	1	-	-	-	-	0.003032	-	-
L C E	1	10	6	-0.22	0.29	0.19	2.15	0.06460	3.824	0.350
	1	10	6	-0.03	0.06	0.04	0.57	0.02751	4.083	0.609
	1	10	6	-	-	-	-	0.02280	-	-
L C E	1	10	1	-0.24	0.29	0.12	2.27	0.04598	4.765	1.291
	1	10	1	-0.03	0.06	0.01	0.61	0.008914	5.896	2.422
	1	10	1	-	-	-	-	0.0006035	-	-

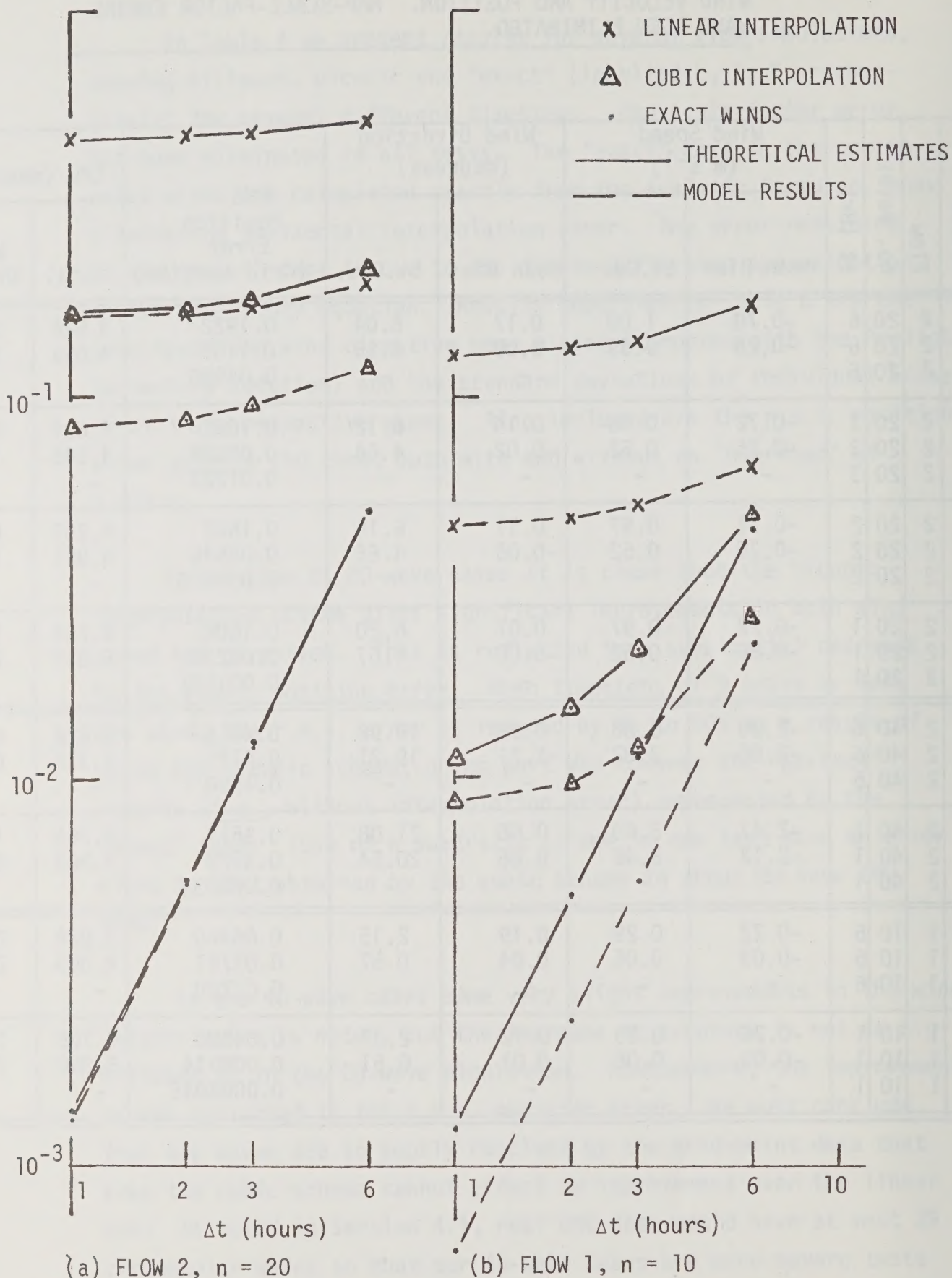


Figure 7. Position error as a function of timestep for two cases with $k = 4$. Linear and cubic schemes for interpolation of winds are compared with results obtained using exact winds.

Therefore we should not be too concerned at the lack of improvement in the bicubic results for 40 waves.

The Flow 1, 10-wave case, proved to be no problem for either linear or cubic scheme, both giving quite small errors in winds and positions. Errors with the cubic scheme, nevertheless, were reduced by 60 to 80%. Differences from a Flow 2, 10-wave simulation are expected to be small, as was shown for the 20-wave case in Section 4.1.

Results from a Flow 1, 20-wave case were comparable to those of the corresponding 85 kPa, 20-wave simulation. Errors with the cubic scheme were reduced by 20-22% compared with the linear scheme.

The results of Table 4 and a few additional points are also plotted in Figure 7. Agreement with upper-bound theoretical estimates is quite good. In the "exact" cases, the slopes of the r.m.s. error is very close to 2 for all flow simulations, indicating agreement with the $(\Delta t)^2$ dependence (Equation A.2). In the case of both linear and cubic interpolations, however, the total error due to interpolation alone, should be independent of Δt (see Equations A.8 and A.9, Appendix 'A'). Our results show slopes which, for the shorter timesteps of 1 and 2 hours are only weakly dependent on Δt , indicating that the temporal truncation error becomes insignificant in comparison with the wind interpolation error. This suggests that it would be futile to attempt to reduce error through use of a variable acceleration scheme as long as wind interpolation errors of these magnitudes are present.

The CPU results, less "overhead", in Table 4 show a relationship which is approximately inversely proportional to (Δt) , regardless of flow or interpolation scheme. The cubic scheme took about 1.7 to 1.9 times as long as the linear scheme.

5. SUMMARY AND CONCLUSIONS

A direct evaluation of the AES trajectory model was performed using specified non-divergent, quasi-realistic wind fields and comparing model calculations with highly accurate solutions for trajectories in those analytic fields.

Sensitivity tests indicated that errors in the model-computed positions were approximately inversely proportional to the wavelength of synoptic-scale waves, in good agreement with theory. When all other sources of error are eliminated, model position errors were shown to be proportional to $(\Delta t)^2$, as predicted by theory. A lower-order finite-difference approximation (zero acceleration) gave errors which were proportional to (Δt) . Errors arising from a variable acceleration scheme were shown to be proportional to $(\Delta t)^2$, with actual magnitudes 40% of the constant acceleration errors. Calculations were not performed with the variable acceleration scheme due to the difficulty of modifying the model. Our results show that temporal truncation errors tend to be dominated by wind interpolation errors, even in the constant acceleration model. Hence the use of a variable acceleration scheme would not give noticeable improvement.

Model errors seemed to be quite insensitive to the convergence criterion employed with the iteration scheme used to solve the finite difference approximation to the trajectory equation.

A small error in the treatment of the map-scale factor in the model was identified. This can be corrected at a cost of only an additional 11% computation time, giving a small improvement in our sensitivity test results. The effect of this correction was examined using real data. It was found that differences in position of up to 100 km after 96 hours appeared in cases of strong meridional circulation.

Theoretical estimates (Appendix 'A') suggest that the largest source of position error in the AES model is that due to horizontal interpolation of winds (excluding from consideration any vertical interpolation errors or those due to boundary-layer parameterization). It was therefore decided to test a bicubic interpolation scheme for comparison with the model's bilinear scheme. For the 40-wave case, the standard 381 km grid is not fine enough to resolve the waves adequately and, consequently, the bicubic scheme did no better than the bilinear. In the case of a 20-wave flow errors with the bicubic scheme were reduced about 50% from those obtained with the bilinear scheme. Reductions of 60 to 80% were noted with the 10-wave flow. These improvements were achieved at the cost of an extra 80% computation time.

Programming changes have been incorporated in a new version of the AES trajectory model which is now available for use. In this version certain programming efficiencies have been incorporated, the map-scale-factor error has been corrected and the option to use bilinear or bicubic horizontal interpolation has been added. Because of the above-mentioned programming improvements, a run with bicubic interpolation now requires about the same time as bilinear interpolation took with the old model version (pre-October 1980).

It is possible to conclude from the present study that increased accuracy is obtained by selection of bicubic interpolation and a shorter timestep. For episode cases this is to be recommended, as computation time is not likely to be a consideration whereas precision is. Most of our test-runs showed significantly less error when the bicubic scheme was used and a further reduction in error when a timestep of 3 hours rather than 6 hours was used. Further shortening of the timestep below 3 hours did not result in much additional accuracy.

For non-episode runs, accuracy may not be as important, though one should perhaps consider the effect of a trajectory just missing a significant emission source due to a position error. Assuming, in these cases, that computation time is an important consideration then it should be borne in mind that an error reduction of 50% or more may be obtained for about 80% additional computing time using the cubic scheme, whereas an error reduction of probably less than 25% is obtained by 100% more computing resulting from a halving of the timestep.

Finally, it should be recalled that the stream function, ψ , was specified as a function of latitude and longitude only. A possible extension to this project would be to make ψ time- and/or height-dependent also, in order to evaluate the accuracy of temporal and vertical interpolation schemes.

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APPENDIX 'A'

ESTIMATES OF MAGNITUDE OF POSITION ERROR IN TRAJECTORY MODELS

As shown in Section 3, total errors associated with temporal truncation in the trajectory equation are:

$$\epsilon_{TOT} = \frac{1}{2} T(\Delta t) \frac{\bar{m}}{\Delta X} U^2 \left[\left(\frac{U_n}{L_n} \right)^2 + \left(\frac{U_k}{L_k} \right)^2 + \left(\frac{\pi}{2} \frac{U}{L_0} \right)^2 \right]^{\frac{1}{2}} \quad (A.1)$$

$$\epsilon_{2TOT} = \frac{5}{12} T(\Delta t)^2 \frac{\bar{m}}{X} U^2 \left[\frac{U_n^2}{L_n^2} + \frac{U_k^2}{L_k^2} + \left(\frac{\pi}{2} \right)^2 \frac{U^2}{L_0^2} \right] \quad (A.3)$$

$$\epsilon_{3TOT} = \frac{2}{5} \epsilon_{2TOT} \quad (A.3)$$

for forward-stepping, constant acceleration and variable acceleration models, respectively. In the above equation Δt is the time-step, $\bar{m}$ is a mean map-scale-factor, ΔX is the grid spacing, U is a characteristic mean zonal wind speed, U_n and U_k are characteristic velocity perturbations, L_0 , L_n and L_k are characteristic length scales appropriate for U , U_n and U_k , respectively and T is the duration of integration.

The error due to assuming that m is constant during the timestep is:

$$\epsilon_{mTOT} = \frac{1}{2} (t) \frac{\Delta m}{\Delta X} U \quad (A.4)$$

where

$$\Delta m = (1 + \sin 60^\circ) \left[\frac{1}{1 + \sin \phi} - \frac{1}{1 + \sin \bar{\phi}} \right] \quad (A.5)$$

is the map-scale-factor error.

An upper bound on errors in the horizontal interpolation of winds is given by:

$$\beta_N = \frac{1/2(-1/2)(-3/2)\dots(1/2-N)}{(N+1)!} \left(\frac{\Delta X}{L}\right)^{N+1} v_p \quad (\text{A.6})$$

where N is the degree of the interpolating polynomial and ΔX is the grid spacing.

Similarly, an upper bound on errors in the temporal interpolation of winds between synoptic observations is expressed

$$\gamma_M = \frac{1/2(-1/2)(-3/2)\dots(1/2-M)}{(M+1)!} (\Delta T)^{M+1} \left(\frac{U}{L}\right)^{M+1} u_p \quad (\text{A.7})$$

where M is the degree of the interpolating polynomial and ΔT is the interval between synoptic observations.

One can translate wind speed errors β_N and γ_M into upper bounds on total position errors in the AES model as follows:

$$\epsilon_{\beta_{N_{TOT}}} = \frac{\bar{m}}{\Delta X} \left| \beta_N^{(1/2)} \right| T \quad (\text{A.8})$$

$$\epsilon_{\gamma_M} = \frac{\bar{m}}{\Delta X} \left| \gamma_M^{(1/2)} \Delta T \right| T \quad (\text{A.9})$$

In Table A.1 we show actual magnitudes of errors which are estimated from the above equations for Flow 2, $k = 4$, $n = 20$ (see Table 1a) with the following assumptions:

$$\phi = 45^\circ \text{N}$$

$$\bar{m} = 1.09, \Delta m = 0.0039$$

$$\Delta X = 381 \text{ km}$$

TABLE A.1 ESTIMATES OF MAGNITUDE OF ERRORS IN THE AES TRAJECTORY MODEL FOR TRAJECTORIES OF 42 HOURS DURATION WITH A TIMESTEP OF 3 HOURS. ASSUMED VALUES OF OTHER PARAMETERS ARE GIVEN IN THE TEXT.

Source of Error	Method	Equation Number(s)	Wind Error each timestep (km/hr)	Position Error (km)	AES Model Characteristics
Trajectory Equation	Forward Stepping	A.1	-	43.8	*
	Constant Acceleration	A.2	-	4.4	
	Variable Acceleration	A.3	-	1.7	
Map-Scale Factor	-	A.4	-	2.8	*
Horizontal Interpolation of Winds (with Constant Acceleration)	Linear (N=1)	A.6, A.8	3.81	160	*
	Quadratic (N=2)	A.6, A.8	1.98	83.4	
	Cubic (N=3)	A.6, A.8	1.34	56.4	
Temporal Interpolation of Winds (with Constant Acceleration)	Linear (M=1)	A.7, A.9	0.088	3.70	*
	Quadratic (M=2)	A.7, A.9	0.028	1.16	
	Cubic (M=3)	A.7, A.9	0.011	0.45	
Wind Observations and Objective Analysis (with Constant Acceleration)	-	-	0.5	21.0	*

$$u_0 = 36 \text{ km hr}^{-1}, U = \cos \phi [2A \sin \phi + D], U_n = B U_0 \sin 2\phi, \\ U_k = C U_0 \sin 2\phi,$$

$$L_0 = 2\pi R \cos \phi / 4, L_n = L_0 / n, L_k = L_0 / k, V_p = n B u_0 \cos \phi, L = L_n,$$

$$\Delta t = 3 \text{ hr}$$

$$T = 42 \text{ hr}$$

$$\Delta T = 6 \text{ hr}$$

$$M = 1, 2, 3$$

$$N = 1, 2, 3$$

The choice of value of Δm is made by assuming northward flow at 36 km hr^{-1} for one timestep (3 hr) giving a displacement of close to one degree latitude. Position errors are obtained in kilometres when Equations (A.1) - (A.4) and (A.8) - (A.9) are multiplied by $\Delta X / \bar{m}$.

Results presented in Table A.1 suggest that the largest source of error, about 44 km for a 42-hour trajectory, is associated with the forward-stepping finite difference approximation to the trajectory equation. This error is reduced to about 4 km in the constant acceleration scheme. A further reduction to about 2 km is achieved with the variable acceleration scheme, but the additional accuracy would seem to be insignificant in comparison with horizontal interpolation errors. It appears, therefore, that the choice of a constant acceleration scheme in the AES model will likely give sufficient accuracy, compared with other sources of error, with the minimum possible computation time.

An upper estimate of about 3 km error due to assuming the map-scale-factor is constant during each three-hour timestep is shown in Table A.1. Thus error caused by inexact treatment of the map-scale-factor in the AES model can be of the same order as temporal truncation error in the trajectory equation. This is especially true in cases of strong meridional flow, with the effect being largest at

low latitudes. This source of error is easily eliminated, through programming changes, with only an 11% increase in computation time (e.g., from 81 to 90s for 2160 trajectories of 96-hour duration).

Estimated upper bounds on total position errors for a 42-hour trajectory arising from horizontal interpolation of winds range from about 160 km for linear interpolation down to about 60 km for cubic interpolation.

It would seem from this analysis that the bilinear scheme presently used in the AES model is potentially the largest source of error in that model. Upgrading to cubic interpolation would probably make the horizontal interpolation errors negligible compared with other errors. This programming change is easily accomplished but it involves an increase of 72% computation time (e.g., from 87 s to 150 s CPU time on the CYBER 76 for 96-hour back-trajectories from 45 points every 6 hours for 8 days.) Thus the more accurate calculations with a cubic interpolation version take 16% less time than the linear version used to take (174 s for the above example) prior to October 1980 when certain programming efficiencies were introduced. Tests with a quadratic scheme gave CPU times similar to those used for the cubic scheme.

Estimated upper bounds on total position errors for a 42-hour trajectory arising from temporal interpolation of winds range from about 4 km linear interpolation down to about 450 m for a cubic scheme. In the AES model, use of a quadratic scheme gives errors of about 1 km which is negligible compared with other errors.

Finally, a rough estimate of grid-point wind velocity component errors of 0.5 km hr^{-1} would lead to position errors of 21 km in 42 hours or 30 km if equivalent errors exist in both wind components. Errors of this magnitude are potentially larger than

those in the AES model, with the possible exception of errors due to the horizontal interpolation of winds using a linear scheme. These estimates again suggest that upgrading to a cubic scheme would mean that all errors arising during calculations with the AES model would be less than those inherent in the wind data. This is a desirable objective, the source of largest errors being beyond the control of the modeller and further model refinements being unlikely to produce improved results.

*Three Dark Figures
Making the Weather
In Folk, in Myth, in Legend,
A threefold test.
Shiva, Vishnu, Brahmin.
Father, Son, Holy Ghost.
Body, Mind, Spirit.
Triune, Triumvirate, Tribunal.
One is Isolate
Two is divisive
Three is Peace.
Three is Torment.
Three is Potent.
Power, Power, Power.
Air, Fire, Water.
Three Dark Figures,
Making the Weather.*

Ron Baird, Sculptor